THE FIRST AND SECOND VARIATION OF THE TOTAL ENERGY OF CLOSED DUPLEX DNA IN PLANAR CASE

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DNA's shape mostly lies on its total energy F. Its corresponding equilibrium shape equations can be got by classical variation method: letting the first energy variation $\delta^{(1)}F = 0$. Here we not only provide the first variation $\delta^{(1)}F$ but also give the second variation $\delta^{(2)}F$ in planar case. Moreover, the general shape equations of DNA are obtained and a mistake in [Zhang, *et al. Phys. Rev. E* **70** 051902 (2004)] is pointed out.

1. Introduction

Closed duplex DNA molecules often have complex configurations, such as supercoil, and those structures play an important role in gene regulation.[1] Theoretical analysis about those configurations are based on the elastic rod theory. In 1859, Kirchhoff given the equilibrium shape equations of thin elastic rod and his methods has been generally used to describe the holistic conformations of duplex DNA.[2−5] Benham[2] treated a homogeneous isotropic rod of the DNA by Kirchhoff analogy and gave some possible shapes. As for the closed duplex DNA molecules, its equilibrium equations are obtained [6], and considerable results are attained.[7−11]

Following the development of modern experimental techniques, such as optical tweezers,[12] micromanipulation,[13−15] and other techniques,[16−18] researchers are presented with more opportunities to probe into the microstructure of individual great molecule than ever before. The ever growing volume of experimental data provides us with the probabilities to improve the existing theoretical models.

Recently, considering the microcosmic configurations of DNA, more practical models, such as the anisotropic model[19] are put forward, and new energy terms are introduced,[20−24] and new methods, such as Monte Carlo simulation[20,25] and path integral,[21] are adopted. Due to those improved theories, some theoretical results are highly consistent with the experimental values.[21,24]

The geometrical configuration of duplex DNA is shown in Fig.1. The axis of the molecule can be written as $\mathbf{R}(s)$ parameterized by the arclength s. The total energy of a simple elastic model for the closed duplex DNA can be written as [9]

$$F = \oint \left(\frac{A}{2} K^2 + B\tau \right) ds, \tag{1}$$

where $K = K(s)$ and $\tau = \tau(s)$ are the curvature and torsion of the axis $\mathbf{R}(s)$. A and B are the bending rigidity and torsional rigidity, respectively. Some researchers also choose a simpler model without the torsional term.[26]

This letter is composed as follows. In Sec. **2**, we will get the equilibrium shape equations of closed duplex DNA by variation theory in its nature coordinates system. In Sec. **3**, a general model is considered and its equilibrium shape equations are attained. In Sec. **4**, we give the second variation $\delta^{(2)}F$ in planar case. Finally, a short discussion is given in Sec. **5**.

2. Classical Equilibrium Shape Equations of Closed Duplex DNA

For a more general case, we choose the total energy of DNA

$$F = \oint \left[\frac{A}{2} (K - C_0)^2 + B(\tau - T_0) \right] ds + \lambda \oint ds, \tag{2}$$

where C_0 and T_0 are two constants, and we call them spontaneous curvature and spontaneous tension respectively, and λ is a Lagrangian multiplier which can be taken as the tensile rigidity. Fig. 1 shows a fragment of $\mathbf{R}(s)$ in the

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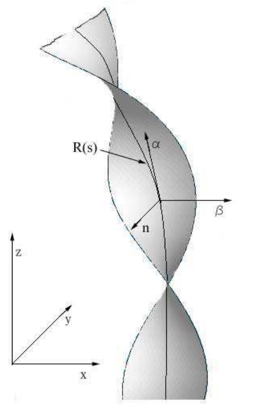

FIG. 1: The geometrical configuration of duplex DNA molecule. The central line of the ribbon follows the molecular axis with coordinates $\mathbf{R}(s)$ parameterized by the arclength s. A nature coordinates is defined: the tangent vector $\boldsymbol{\alpha}$, the main normal vector $\mathbf{n}$ and the vice-normal vector $\boldsymbol{\beta}$

orthogonal coordinates system (x, y, z). Meantime, a nature (local) coordinates can be described as

$$(\boldsymbol{\alpha}, \mathbf{n}, \boldsymbol{\beta}). \tag{3}$$

Where, $\boldsymbol{\alpha} = \dot{\mathbf{R}}$ is the tangent vector (an overdot denotes differential with respect to s), $\mathbf{n} = \ddot{\mathbf{R}}/K$ is the main normal vector and $\boldsymbol{\beta} = \boldsymbol{\alpha} \times \mathbf{n}$ is the vice-normal vector. Between those unit vectors and K and τ, there are the Frenet formulaes

$$\dot{\boldsymbol{\alpha}} = K(s)\mathbf{n}, \tag{4}$$
$$\dot{\mathbf{n}} = -K(s)\boldsymbol{\alpha} + \tau(s)\boldsymbol{\beta}, \tag{5}$$
$$\dot{\boldsymbol{\beta}} = -\tau(s)\mathbf{n}. \tag{6}$$

The equilibrium shape equations will be extracted by analyzing the first variation

$$\delta^{(1)}F = 0. \tag{7}$$

Letting $g = \mathbf{R}_{,x} \cdot \mathbf{R}_{,x}$ ($\mathbf{R}_{,x} = \frac{d\mathbf{R}}{dx}$), we have $ds = \sqrt{g}dx$. So, Eq. (7) induced

$$\oint \Big\{ \Big[A(K - C_0)\delta^{(1)}K + B\delta^{(1)}\tau \Big] \sqrt{g} + \left[\frac{A}{2}(K - C_0)^2 + B(\tau - T_0) + \lambda \right] \delta^{(1)}(\sqrt{g}) \Big\} dx = 0. \tag{8}$$

Before we get the equilibrium shape equations, some useful identical equations should be calculated (see appendix A).

The $\mathbf{R}(s)$ under small perturbations can be written as

$$\mathbf{R}^{'}(s) = \mathbf{R}(s) + \psi(s)\mathbf{n} + \varphi(s)\boldsymbol{\beta}, \tag{9}$$

where $\psi(s)$ and $\varphi(s)$ are two small smooth functions. We get

$$\delta\mathbf{R} = \mathbf{R}^{'} - \mathbf{R} = \psi\mathbf{n} + \varphi\boldsymbol{\beta} \tag{10}$$
$$\delta\mathbf{R}_{,x} = (\delta\mathbf{R})_{,x} = \sqrt{g}(\delta\mathbf{R})_{,s} = \sqrt{g}(\dot{\psi}\mathbf{n} + \psi\dot{\mathbf{n}} + \dot{\varphi}\boldsymbol{\beta} + \varphi\dot{\boldsymbol{\beta}}) \tag{11}$$

and

$$\begin{aligned} \delta g &= (\mathbf{R}_{,x} + \delta\mathbf{R}_{,x}) \cdot (\mathbf{R}_{,x} + \delta\mathbf{R}_{,x}) - \delta\mathbf{R}_{,x} \cdot \delta\mathbf{R}_{,x} \\ &= 2\mathbf{R}_{,x} \cdot \delta\mathbf{R}_{,x} + \delta\mathbf{R}_{,x} \cdot \delta\mathbf{R}_{,x} = g[2\dot{\mathbf{R}} \cdot (\delta\mathbf{R})_{,s} + (\delta\mathbf{R})_{,s} \cdot (\delta\mathbf{R})_{,s}] \\ &= -2gK\psi + g\left[\dot{\psi}^2 + \psi^2(K^2 + \tau^2) + \dot{\varphi}^2 + \varphi^2\tau^2 + 2(\psi\dot{\varphi} - \dot{\psi}\varphi)\tau\right]. \end{aligned} \tag{12}$$

Consequently, we have

$$\begin{aligned}
\delta g^{\frac{1}{2}} &= (g+\delta g)^{\frac{1}{2}} - g^{\frac{1}{2}} = g^{\frac{1}{2}}\left[\frac{1}{2}\left(\frac{\delta g}{g}\right) - \frac{1}{8}\left(\frac{\delta g}{g}\right)^2 + \cdots\right] \\
&= -g^{\frac{1}{2}}K\psi + \frac{1}{2}g^{\frac{1}{2}}\left[\dot{\psi}^2 + (\psi^2+\varphi^2)\tau^2 + \dot{\varphi}^2 + 2(\psi\dot{\varphi} - \dot{\psi}\varphi)\tau\right] + O(3), \qquad (13)
\end{aligned}$$

$$\begin{aligned}
\delta g^{\frac{-1}{2}} &= (g+\delta g)^{\frac{-1}{2}} - g^{\frac{-1}{2}} = g^{\frac{-1}{2}}\left[-\frac{1}{2}\left(\frac{\delta g}{g}\right) + \frac{3}{8}\left(\frac{\delta g}{g}\right)^2 + \cdots\right] \\
&= g^{\frac{-1}{2}}K\psi - \frac{1}{2}g^{\frac{-1}{2}}\left[\dot{\psi}^2 + (\psi^2+\varphi^2)\tau^2 + \dot{\varphi}^2 - 2\psi^2K^2 + 2(\psi\dot{\varphi} - \dot{\psi}\varphi)\tau\right] \\
&\quad + O(3). \qquad (14)
\end{aligned}$$

Where $O(3)$ means the third and higher orders of ψ and φ. We can also attain

$$\begin{aligned}
\delta\dot{\mathbf{R}} &= \delta(g^{\frac{-1}{2}}\mathbf{R}_{,x}) = (g^{\frac{-1}{2}} + \delta g^{\frac{-1}{2}})(\mathbf{R}_{,x} + \delta\mathbf{R}_{,x}) - \dot{\mathbf{R}} \\
&= (1 + g^{\frac{1}{2}}\delta g^{\frac{-1}{2}})(\delta\mathbf{R})_{,s} + g^{\frac{1}{2}}\dot{\mathbf{R}}\delta g^{\frac{-1}{2}} \qquad (15)
\end{aligned}$$

This conclusion can be generalized to an arbitrate function $\mathbf{V} = \mathbf{V}(s)$, which satisfies

$$\delta\dot{\mathbf{V}} = (1 + g^{\frac{1}{2}}\delta g^{\frac{-1}{2}})(\delta\mathbf{V})_{,s} + g^{\frac{1}{2}}\dot{\mathbf{V}}\delta g^{\frac{-1}{2}} \qquad (16)$$

Submitting (11) and (14) into (15), we get

$$\begin{aligned}
\delta\dot{\mathbf{R}} &= K\psi\dot{\mathbf{R}} + \dot{\psi}\mathbf{n} + \psi\dot{\mathbf{n}} + \dot{\varphi}\boldsymbol{\beta} + \varphi\dot{\boldsymbol{\beta}} + K\psi(\dot{\psi}\mathbf{n} + \psi\dot{\mathbf{n}} + \dot{\varphi}\boldsymbol{\beta} + \varphi\dot{\boldsymbol{\beta}}) \\
&\quad -\frac{1}{2}\dot{\mathbf{R}}\left[\dot{\psi}^2 + \dot{\varphi}^2 + (\psi^2+\varphi^2)\tau^2 - 2\psi^2K^2 + 2(\psi\dot{\varphi} - \dot{\psi}\varphi)\tau\right] + O(3). \qquad (17)
\end{aligned}$$

Using (16), we have

$$\delta\ddot{\mathbf{R}} = (1 + g^{\frac{1}{2}}\delta g^{\frac{-1}{2}})(\delta\dot{\mathbf{R}})_{,s} + g^{\frac{1}{2}}\ddot{\mathbf{R}}\delta g^{\frac{-1}{2}}. \qquad (18)$$

Insetting (14) and (17) into (18) we get

$$\begin{aligned}
\delta\ddot{\mathbf{R}} &= 2K\psi\ddot{\mathbf{R}} + \dot{\mathbf{R}}(\dot{K}\psi + K\dot{\psi}) + \ddot{\psi}\mathbf{n} + \psi\ddot{\mathbf{n}} + 2\dot{\psi}\dot{\mathbf{n}} + \ddot{\varphi}\boldsymbol{\beta} + \varphi\ddot{\boldsymbol{\beta}} + 2\dot{\varphi}\dot{\boldsymbol{\beta}} \\
&\quad + K\psi\left[2\ddot{\psi}\mathbf{n} + 2\psi\ddot{\mathbf{n}} + 2\varphi\ddot{\boldsymbol{\beta}} + 2\ddot{\varphi}\boldsymbol{\beta} + 4\dot{\psi}\dot{\mathbf{n}} + 4\dot{\varphi}\dot{\boldsymbol{\beta}} + K\psi\ddot{\mathbf{R}} + (\dot{K}\psi + K\dot{\psi})\dot{\mathbf{R}}\right] \\
&\quad - \ddot{\mathbf{R}}\left[\dot{\psi}^2 + \dot{\varphi}^2 + (\psi^2+\varphi^2)\tau^2 - 2K^2\psi^2 + 2(\psi\dot{\varphi} - \dot{\psi}\varphi)\tau\right] \\
&\quad + (\dot{K}\psi + K\dot{\psi})(\dot{\psi}\mathbf{n} + \psi\dot{\mathbf{n}} + \dot{\varphi}\boldsymbol{\beta} + \varphi\dot{\boldsymbol{\beta}}) \\
&\quad - \dot{\mathbf{R}}\Big[\tau\dot{\tau}(\psi^2+\varphi^2) - 2K\dot{K}\psi^2 - 2K^2\psi\dot{\psi} + \dot{\tau}(\psi\dot{\varphi} - \dot{\psi}\varphi) + \tau^2(\psi\dot{\psi} + \varphi\dot{\varphi}) \\
&\quad + \dot{\psi}\ddot{\psi} + \dot{\varphi}\ddot{\varphi} + \tau(\psi\ddot{\varphi} - \ddot{\psi}\varphi)\Big] + O(3). \qquad (19)
\end{aligned}$$

Noting $K^2 = \ddot{\mathbf{R}}\cdot\ddot{\mathbf{R}}$, we have

$$\delta^{(1)}K = (\ddot{\mathbf{R}}\cdot\delta^{(1)}\ddot{\mathbf{R}})/K. \qquad (20)$$

Submitting (19) into (20) and using the identical equations in appendix A, we attain

$$\delta^{(1)}K = \left(K^2 - \tau^2\right)\psi + \ddot{\psi} - \dot{\tau}\varphi - 2\tau\dot{\varphi}. \qquad (21)$$

Now, we calculate

$$\begin{aligned}
\delta^{(1)}\dot{\mathbf{n}} &= \dot{\mathbf{n}}\sqrt{g}\delta^{(1)}(g^{-1/2}) + g^{-1/2}\left[\delta^{(1)}\left(\frac{\ddot{\mathbf{R}}}{K}\right)\right]_{,x} \\
&= \left[\frac{K\delta^{(1)}\ddot{\mathbf{R}} - \ddot{\mathbf{R}}\delta^{(1)}K}{K^2}\right]_{,s} + \dot{\mathbf{n}}K\psi. \qquad (22)
\end{aligned}$$

Submitting (19) and (21) into (22), we get $\delta^{(1)}\dot{\mathbf{n}}$. Then, using the identic equations in appendix A, the following useful term can be attained

$$\begin{aligned}\dot{\mathbf{n}}\cdot\delta^{(1)}\dot{\mathbf{n}} &= K^3\psi + K\left(\tau^2\psi - \dot{\tau}\varphi - \tau\dot{\varphi} + \ddot{\psi}\right)\\ &+K^{-1}\tau\left[\ddot{\tau}\psi - \tau^2\dot{\varphi} + 3\dot{\tau}\dot{\psi} + 2\tau(\ddot{\psi} - \dot{\tau}\varphi) + \varphi^{(3)}\right]\\ &+K^{-2}\dot{K}\tau\left(\tau^2\varphi - \dot{\tau}\psi - 2\tau\dot{\psi} - \ddot{\varphi}\right).\end{aligned} \tag{23}$$

Considering $\dot{\mathbf{n}}\cdot\dot{\mathbf{n}} = K^2 + \tau^2$, we have

$$\delta^{(1)}\tau = \frac{\dot{\mathbf{n}}\cdot\delta^{(1)}\dot{\mathbf{n}} - K\delta^{(1)}K}{\tau}. \tag{24}$$

Taking (21) and (23) into (24), we get

$$\begin{aligned}\delta^{(1)}\tau &= K(2\tau\psi + \dot{\varphi}) + K^{-2}\dot{K}\left(\tau^2\varphi - \dot{\tau}\psi - 2\tau\dot{\psi} - \ddot{\varphi}\right)\\ &+K^{-1}\left[\ddot{\tau}\psi + 3\dot{\tau}\dot{\psi} - \tau^2\dot{\varphi} + \varphi^{(3)} + 2\tau\left(\ddot{\psi} - \varphi\dot{\tau}\right)\right].\end{aligned} \tag{25}$$

Submitting (13), (21) and (25) into (8), we attain

$$\begin{aligned}\delta^{(1)}F &= \oint\Big\{-K\psi\left[\frac{A}{2}(K-C_0)^2 + B(\tau - T_0) + \lambda\right]\\ &+A(K-C_0)\left[\left(K^2-\tau^2\right)\psi - \dot{\tau}\varphi - 2\tau\dot{\varphi} + \ddot{\psi}\right]\\ &+BK(2\tau\psi + \dot{\varphi}) + BK^{-2}\dot{K}\left(\tau^2\varphi - \dot{\tau}\psi - 2\tau\dot{\psi} - \ddot{\varphi}\right)\\ &+BK^{-1}\left[\ddot{\tau}\psi + 3\dot{\tau}\dot{\psi} - \tau^2\dot{\varphi} + \varphi^{(3)} + 2\tau\left(\ddot{\psi} - \dot{\tau}\varphi\right)\right]\Big\}ds.\end{aligned} \tag{26}$$

If perturbation is only on the main normal direction ($\varphi = 0$), we have

$$\begin{aligned}F_0 &= \frac{1}{2}A\left(K^3 + 2C_0\tau^2 - KC_0^2 - 2K\tau^2\right) - K\left(\lambda - B\tau - BT_0\right)\\ &+BK^{-2}(K\ddot{\tau} - \dot{K}\dot{\tau}),\\ F_1 &= BK^{-2}(3K\dot{\tau} - 2\dot{K}\tau),\\ F_2 &= A(K-C_0) + 2BK^{-1}\tau,\\ \delta^{(1)}F &= \oint\left(F_0\psi + F_1\dot{\psi} + F_2\ddot{\psi}\right)ds.\end{aligned} \tag{27}$$

For two smooth functions $Q = Q(s)$ and $P = P(s)$, there is

$$\oint Q^{(n)}Pds = (-1)^n\oint P^{(n)}Qds, \tag{28}$$

where $n = 1, 2, 3\cdots$. Using (28), (27) can be changed into

$$\delta^{(1)}F = \oint\left[\frac{1}{2}AK^3 - \frac{1}{2}K\left(AC_0^2 + 2\lambda - 2BT_0 - 2B\tau + 2A\tau^2\right) + A\left(C_0\tau^2 + \ddot{K}\right)\right]\psi ds. \tag{29}$$

Because ψ is an arbitrary function, so the equilibrium shape equation under main normal perturbation is

$$AK^3 - K(AC_0^2 + 2\lambda - 2BT_0 - 2B\tau + 2A\tau^2) + 2A(C_0\tau^2 + \ddot{K}) = 0. \tag{30}$$

Another equilibrium shape equation under vice-normal perturbation can be obtained through the former way. Choosing $\psi = 0$, (26) can be simplified as

$$\begin{aligned}F_0 &= BK^{-2}\dot{K}\tau^2 + 2BK^{-1}\dot{\tau}\tau - A(K-C_0)\dot{\tau},\\ F_1 &= K(B - 2A\tau) + 2AC_0\tau - BK^{-1}\tau^2,\\ F_2 &= -BK^{-2}\dot{K},\\ F_3 &= BK^{-1},\\ \delta^{(1)}F &= \oint\left(F_0\varphi + F_1\dot{\varphi} + F_2\ddot{\varphi} + F_3\varphi^{(3)}\right)ds.\end{aligned} \tag{31}$$

The corresponding equilibrium shape equation obtained by $F_0 - \frac{dF_1}{ds} + \frac{d^2F_2}{ds^2} - \frac{d^3F_3}{ds^3} = 0$ is

$$A(K - C_0)\dot{\tau} - (B - 2A\tau)\dot{K} = 0. \tag{32}$$

Eq. (32) can be changed into the following state:

$$(K - C_0)^2(2\tau - Q) = C, \tag{33}$$

where $Q = B/A$, and C is a constant. When $C_0 = T_0 = \lambda = 0$, similar equations are attained and an elliptic function solution is found in Ref. [6]. In particular, if $\mathbf{R}(s)$ is a planar line ($\tau = B = T_0 = 0$), only Eq. (30) is valid and is reduced to an elliptic different equation

$$2A\ddot{K} + AK^3 - (AC_0^2 + 2\lambda)K = 0. \tag{34}$$

A similar equation was discussed in vesicle research.[27]

Here, two special cases should be taken into account. First, there is a ring solution to Eq. (34):

$$K = 1/r = \sqrt{C_0^2 + 2\lambda/A}, \tag{35}$$

where r is the the ring's radius. If there is stable planar ring DNAs, we need

$$C_0^2 + 2\lambda/A > 0. \tag{36}$$

Second, it might have isolated inflexion points in the two shape equations at $s = s_0$, if

$$K(s_0) = C_0. \tag{37}$$

When $C_0 = 0$, this problem is discussed in Ref. [6]. At the inflexion points, DNA's shape may has uncertain behavior. Let's see an example. Choosing $C = 0$ in (33) and supposing $R(s)$ is a solution of Eqs. (30) and (33), then, one can find that if there is a point $s = s_0$ in $R(s)$ satisfies $K(s_0) = C_0$, Eq. (33) will lose the constraint of τ and there is only Eq. (30) which needs to be satisfied. In this case, Eq. (30) is easy to be satisfied, because it has two variables: K and τ. Therefore, we can expect that DNA's shape changes variably at its inflexion points.

3. General Shape Equations

It is known that the curvature K and torsion τ are two characteristic parameters which can determine a line's shape. Recently, new energy terms are introduced[20−24] in DNA's total energy. Those new energy terms will influence DNA's shape through changing its local curvature and tension. Moreover, DNA's total energy can be written as the sum of the elastic energy of its two molecular lines: $F_i = \oint[AK^2(s_i) + B\tau^2(s_i)]ds$ ($i = 1, 2$) (see Ref. [4]). Where s_i is the arclength of one of DNA's molecular lines. Clearly, we can choose one of DNA's molecular lines to determine its shape and attain its shape equations by letting $\delta^{(1)}F_i = 0$.

Here, we suppose that those new energy terms can be expressed by curvature and tension, and we choose the total energy of closed DNA

$$F = \oint f(K, \tau)ds, \tag{38}$$

where $f(K, \tau)$ is a function with two variables K and τ. Similar method is adopted in vesicle research.[28,29] By the former way we have discussed the first order variation of total energy, that is

$$\delta^{(1)}F = \oint[(f_{,K}\delta^{(1)}K + f_{,\tau}\delta^{(1)}\tau)\sqrt{g} + f\delta^{(1)}(\sqrt{g})]dx, \tag{39}$$

where $f_{,K} = \frac{\partial f}{\partial K}$. Submitting (13), (21) and (25) into (39), we get

$$\begin{aligned}
F_0 &= -K\psi, \\
F_1 &= \left(K^2 - \tau^2\right)\psi - \dot{\tau}\varphi - 2\tau\dot{\varphi} + \ddot{\psi}, \\
F_2 &= K(2\tau\psi + \dot{\varphi}) + K^{-2}\dot{K}\left(\tau^2\varphi - \dot{\tau}\psi - 2\tau\dot{\psi} - \ddot{\varphi}\right) \\
&\quad + K^{-1}\left[3\dot{\tau}\dot{\psi} - \tau^2\dot{\varphi} + \ddot{\tau}\psi + \varphi^{(3)} + 2\tau\left(\ddot{\psi} - \dot{\tau}\varphi\right)\right], \\
\delta^{(1)}F &= \oint\left(F_0 f + F_1 f_{,K} + F_2 f_{,\tau}\right)ds.
\end{aligned} \tag{40}$$

Perturbation only on main normal direction ($\varphi = 0$) induces

$$\begin{aligned}
F_0 &= \left(K^2 - \tau^2\right) f_{,K} + K^{-2}\left(2K^3\tau - \dot{K}\dot{\tau} + K\ddot{\tau}\right) f_{,\tau} - Kf, \\
F_1 &= K^{-2}(3K\dot{\tau} - 2\dot{K}\tau) f_{,\tau}, \\
F_2 &= f_{,K} + 2K^{-1}\tau f_{,\tau}, \\
\delta^{(1)} F &= \oint \left(F_0\psi + F_1\dot{\psi} + F_2\ddot{\psi}\right) ds. \qquad (41)
\end{aligned}$$

The corresponding equilibrium shape equation is

$$\begin{aligned}
&\frac{d^2}{ds^2}(f_{,K} + 2K^{-1}\tau f_{,\tau}) - \frac{d}{ds}\left[K^{-2}(3K\dot{\tau} - 2\dot{K}\tau) f_{,\tau}\right] \\
&+ \left(K^2 - \tau^2\right) f_{,K} + K^{-2}\left(2K^3\tau - \dot{K}\dot{\tau} + K\ddot{\tau}\right) f_{,\tau} - Kf = 0. \qquad (42)
\end{aligned}$$

If perturbation is on vice-normal direction ($\psi = 0$), (40) is simplified as

$$\begin{aligned}
F_0 &= K^{-2}\tau(\dot{K}\tau - 2K\dot{\tau}) f_{,\tau} - \dot{\tau} f_{,K}, \\
F_1 &= K^{-1}\left(K^2 - \tau^2\right) f_{,\tau} - 2\tau f_{,K}, \\
F_2 &= -K^{-2}\dot{K} f_{,\tau}, \\
F_3 &= K^{-1} f_{,\tau}, \\
\delta^{(1)} F &= \oint \left(F_0\varphi + F_1\dot{\varphi} + F_2\ddot{\varphi} + F_3\varphi^{(3)}\right) ds. \qquad (43)
\end{aligned}$$

The corresponding equilibrium shape equation is

$$\begin{aligned}
&\frac{d^3}{ds^3}\left(K^{-1} f_{,\tau}\right) + \frac{d^2}{ds^2}\left(K^{-2}\dot{K} f_{,\tau}\right) + \frac{d}{ds}\left[K^{-1}\left(K^2 - \tau^2\right) f_{,\tau} - 2\tau f_{,K}\right] \\
&\qquad - K^{-2}\tau(\dot{K}\tau - 2K\dot{\tau}) f_{,\tau} + \dot{\tau} f_{,K} = 0. \qquad (44)
\end{aligned}$$

Eqs. (42) and (44) are the general equilibrium shape equations for closed DNA. Comparing Eqs.(41) and (43) with Eqs.(6) and (7) in Ref. [30] respectively, we find that Eq. (42) is equal to Eq. (6) in Ref. [30] ($\alpha(s) = \alpha_s(s) = 0$). But Eq. (43) is not equal to Eq. (7) in Ref. [30]. Acutely, the mistakes in Ref. [31] induce the incorrect result in Refs. [31] and [30] (see appendix B). Moreover, similar correct equations are also shown in Ref. [32] (Eqs.(16) and (17)), in Ref. [33] (Eqs.(1) and (2)) and in Ref. [34] (Eqs.(77) and (78)).

4. Second Variation in planar case

We know that stability condition needs the second variation $\delta^{(2)}F > 0$, so we want to get $\delta^{(2)}F$ by the former way. For simplify, we only consider the planar case with the energy $F = \oint (K^2 + \lambda) ds$. Consider $K^2 = \ddot{\mathbf{R}} \cdot \ddot{\mathbf{R}}$, there is

$$\delta K^2 = 2\ddot{\mathbf{R}} \cdot \delta\ddot{\mathbf{R}} + \delta\ddot{\mathbf{R}} \cdot \delta\ddot{\mathbf{R}}. \qquad (45)$$

Submitting (19) into the above equation, we get

$$\begin{aligned}
\delta K^2 &= 2\ddot{\mathbf{R}} \cdot \delta\ddot{\mathbf{R}} + \delta\ddot{\mathbf{R}} \cdot \delta\ddot{\mathbf{R}} \\
&= 2K(K^2\psi - \tau^2\psi - \dot{\tau}\varphi - 2\tau\dot{\varphi} + \ddot{\psi}) + 3K^4\psi^2 + \tau^4(\varphi^2 + \psi^2) \\
&\quad + (\varphi^2 + \psi^2)\dot{\tau}^2 + 4\tau^3(\psi\dot{\varphi} - \dot{\psi}\varphi) + 2\dot{K}K\psi(\dot{\psi} - \tau\varphi) \\
&\quad + 2\dot{\tau}(\psi\ddot{\varphi} - \ddot{\psi}\varphi) + \ddot{\psi}^2 + \ddot{\varphi}^2 - K^2\Big[\tau^2(\varphi^2 + 8\psi^2) + 6\dot{\tau}\psi\varphi \\
&\quad + 16\tau\psi\dot{\varphi} + 2\dot{\varphi}^2 - \dot{\psi}^2 - 6\ddot{\psi}\psi\Big] + 2\tau^2(2\dot{\psi}^2 + 2\dot{\varphi}^2 - \ddot{\psi}\psi - \ddot{\varphi}\varphi) \\
&\quad + 4\tau\Big[\dot{\tau}(\dot{\psi}\psi + \dot{\varphi}\varphi) + \dot{\psi}\ddot{\varphi} - \ddot{\psi}\dot{\varphi}\Big] + O(3) \qquad (46)
\end{aligned}$$

Allying (13), we get the second variation of DNA's energy (note $\tau = \varphi = 0$)

$$
\begin{aligned}
\delta^{(2)} F &= \oint \left[(K^2+\lambda)\delta^{(2)}\sqrt{g} + \sqrt{g}\delta^{(2)}K^2 + \delta^{(1)}\sqrt{g}\delta^{(1)}K^2 \right] dx \\
&= \oint \left[\frac{1}{2}(3K^2+\lambda)\dot{\psi}^2 + 4K^2\psi\ddot{\psi} + K^4\psi^2 + 2K\dot{K}\psi\dot{\psi} + \ddot{\psi}^2 \right] ds. \qquad (47)
\end{aligned}
$$

The above equation can be used to analysis the stability of DNA in planar case. For instance, it's easy to find that straight line $K = 0$ is a stable solution of Eq. (34) if $\lambda \geq 0$.

5. Discussion

In Sec. **2**, we give the DNA's shape equations which contain two special constants: C_0 and T_0. But what are their physical meaning? Maybe we can take them as the influence of the environmental factors or other complications. For example, compared with vesicle research, those two constants can be attributed to the donation of electric potential on DNA.

In (47) we only give $\delta^{(2)}F$ in planar case, if we want to get $\delta^{(2)}F$ in a more general case, $\delta^{(2)}K$ and $\delta^{(2)}\tau$ should be obtained formerly. For instance, if we consider

$$
\delta X^n = nX^{n-1}\delta X + \frac{n(n-1)}{2!}(\delta X)^2 + \cdots, \qquad (48)
$$

where $X = X(s)$ is a scalar function of s, and n is a constant, we can attain all δK^n terms by using Eq. (46). Moreover, using (16), all $\delta K^{(m)}$ ($K^{(m)} = \frac{d^m K}{ds^m}$, $m = 1, 2\cdots$) terms can be obtained. Finally, because attaining $\delta\tau^{(2)}$ needs a tedious calculation, we will show it and discuss $\delta^{(2)}F$ in another paper.

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APPENDIX A

In this appendix, we show some useful identical equations which can be attained easily.

$$\dot{\mathbf{n}}\cdot\dot{\mathbf{R}} = -K, \tag{A1}$$
$$\dot{\mathbf{n}}\cdot\ddot{\mathbf{R}} = 0, \tag{A2}$$
$$\dot{\mathbf{n}}\cdot\mathbf{R}^{(3)} = K^3+\tau^2 K, \tag{A3}$$
$$\dot{\mathbf{n}}\cdot\mathbf{R}^{(4)} = 3\dot{K}K^2+\tau(2\dot{K}\tau+K\dot{\tau}), \tag{A4}$$
$$\dot{\mathbf{n}}\cdot\boldsymbol{\beta} = \tau, \tag{A5}$$
$$\dot{\mathbf{n}}\cdot\dot{\boldsymbol{\beta}} = 0, \tag{A6}$$
$$\dot{\mathbf{n}}\cdot\ddot{\boldsymbol{\beta}} = -\tau^3-K^2\tau, \tag{A7}$$
$$\dot{\mathbf{n}}\cdot\boldsymbol{\beta}^{(3)} = -K\dot{K}\tau-2K^2\dot{\tau}-3\tau^2\dot{\tau}, \tag{A8}$$
$$\dot{\mathbf{n}}\cdot\dot{\mathbf{n}} = K^2+\tau^2, \tag{A9}$$
$$\dot{\mathbf{n}}\cdot\ddot{\mathbf{n}} = K\dot{K}+\tau\dot{\tau}, \tag{A10}$$
$$\dot{\mathbf{n}}\cdot\mathbf{n}^{(3)} = K\ddot{K}+\tau\ddot{\tau}-(K^2+\tau^2)^2, \tag{A11}$$
$$\ddot{\mathbf{n}}\cdot\ddot{\mathbf{n}} = \dot{K}^2+\dot{\tau}^2+(K^2+\tau^2)^2. \tag{A12}$$

APPENDIX B

In this appendix, we point out a mistake in Ref. [31]. Comparing this letter with Ref. [31], we find that they are similar work. Here we use ψ and φ to determine the perturbations on the main normal direction $\mathbf{n}$ and the the vice-normal direction $\boldsymbol{\beta}$, respectively. (Actually, there should be perturbation on the tangent direction $\boldsymbol{\alpha}$, but we find that it will not induces any new shape equation, so we ignore it deliberately.) In Ref. [31], there are three corresponding perturbation functions: ε_1 on the tangent direction $\boldsymbol{\alpha}$, ε_2 on the main normal direction $\mathbf{n}$ and ε_3 on the vice-normal direction $\boldsymbol{\beta}$. Clearly, there are the relationships

$$\psi=\varepsilon_2,\ \varphi=\varepsilon_3. \tag{B1}$$

Comparing Eq. (25) with Eq. (2.27) in Ref. [31], we find they are not equal. There are two mistakes in Eq. (2.27) in Ref. [31] that the first term $K^2\varepsilon_3$ in the first bracket should be changed as $\tau^2\varepsilon_3$, and the $-\varepsilon_3^{(3)}$ term should be $\varepsilon_3^{(3)}$. The correct $\delta^{(1)}\tau$ in Eq. (2.27) in Ref. [31] should be

$$\begin{aligned}\delta^{(1)}\tau \;=\; & \frac{1}{K^2}\Big\{\dot{K}(\tau^2\varepsilon_3-\dot{\tau}\varepsilon_2-2\tau\dot{\varepsilon}_2-\ddot{\varepsilon}_3)\\ & +K\left[2K^2\tau\varepsilon_2+\dot{\tau}(-2\tau\varepsilon_3+3\dot{\varepsilon}_2)+(K^2-\tau^2)\dot{\varepsilon}_3+\ddot{\tau}\varepsilon_2+2\tau\ddot{\varepsilon}_2+\varepsilon_3^{(3)}\right]\Big\}.\end{aligned} \tag{B2}$$

One can find that the above equation is equal to Eq. (25) (note $\varepsilon_1 = 0$). It is this mistake that induces the incorrect shape equations: Eq. (2.32) in Ref. [31] and Eq. (7) in Ref. [30].